

Quasiparticles beyond the Fermi liquid and heavy fermion criticality

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We give a self-consistent theory of the scale dependent effective mass enhancement m^*/m of quasiparticles by 3D antiferromagnetic (AFM) spin fluctuations in the presence of disorder at an AFM quantum critical point. The coupling of fermionic and bosonic degrees of freedom in the critical regime is described in terms of a critical quasiparticle theory. Using the fact that even in the “non-Fermi liquid” regime the quasiparticle width does not exceed the quasiparticle energy, we adopt relations from Fermi liquid theory to determine the dependence of the spin fluctuation spectrum on m^*/m , from which the self energy and hence m^*/m may be calculated. The self-consistent equation for m^*/m has a strong coupling solution provided the initial value is sufficiently large. We argue that in YbRh₂Si₂ (YRS), quasi-2D AFM and/or 3D ferromagnetic Gaussian fluctuations existing over a wide range drive the system into the 3D strongly coupled fluctuation regime. We find critical exponents of the temperature dependence of the specific heat coefficient $\gamma \propto T^{-1/4}$ and of the resistivity $\rho(T) = \rho(0) + AT^{3/4}$ in good agreement with experiments on YbRh₂Si₂ in the temperature range $T < 0.3K$.

Introduction. Quantum phase transitions differ from thermodynamic phase transitions in that temporal fluctuations are of equal importance or may be even dominant compared to spatial fluctuations. Early theories of quantum critical behavior, formulated in the framework of a Ginzburg-Landau-Wilson action of the order parameter field ϕ [1, 2], found that the effective dimension of the corresponding ϕ^4 -field theory is increased to $d_{eff} = d + z$ where d, z are the spatial dimension of the fluctuations and the dynamical critical exponent, respectively. In many cases of interest d_{eff} is above the upper critical dimension, so that the fluctuations are effectively non-interacting and the theory is of the Gaussian type.

However, several metallic compounds exhibit a quantum critical point with non-Gaussian character [3, 4] (for a review see [5]). Many of the systems for which the Gaussian theory is found to fail show strong electronic correlations, as exemplified by a strongly enhanced effective mass ratio m^*/m (heavy fermion systems). One might expect that in such systems it is not possible to integrate out the fermionic degrees of freedom in favor of a purely bosonic theory. Rather, in many cases the fermionic properties, in particular the effective quasiparticle mass, develop critical behavior, which will feed back into the bosonic spectrum. One is then faced with formulating a critical theory of coupled fermionic and bosonic degrees of freedom. Moreover, all signs indicate that such a theory would be in the strong-coupling regime.

Over the past ten years several proposals dealing with this situation have been formulated [6–8]. Some of these scenarios have been developed enough to allow comparison with experimentally observed critical exponents, in particular for CeCu_{5.9}Au_{0.1} and for YbRh₂Si₂ [9, 10].

In this letter, we analyze the behavior near an AFM QCP within a heavy-quasiparticle picture based on the

Anderson lattice model and we refer our results to the heavy fermion compound YbRh₂Si₂ (YRS). When the energy scale T_K of the lattice Kondo effect and that of the onset of the critical regime T_{cr} are as wide apart as they are for YRS, namely $T_K \approx 25K$ and $T_{cr} \approx 0.3K$, we may assume that well below T_K , the Kondo screening and hence the heavy-quasiparticle picture are robust. However, the effect of AFM quantum critical fluctuations leads to a further renormalization of the quasiparticle spectrum, which generates a critical (scaling) behavior of the effective mass [11]. In contrast to other approaches (*e.g.* [10]), we address the non-Gaussian critical region and consider the interaction of the heavy quasiparticles with AFM fluctuations. We shall show that a self-consistent theory of a divergent quasiparticle effective mass generated by interaction with 3D AFM fluctuations is capable of providing a sufficiently accurate account of the critical region as seen experimentally. The interplay of spin fluctuations and fermionic excitations has also been considered in $1/N$ expansion by Abanov and Chubukov [12] and a renormalization group formulation has been given by Metitski and Sachdev [13].

The above scenario depends sensitively on the detailed nature of spin fluctuations in a given system. For example, 3D AFM fluctuations do not lead to true critical behavior, *i.e.* a Gaussian fluctuation theory is applicable [1, 2], provided the effective mass ratio is not too large. We argue below that in YRS one has a wide region of quasi-2D antiferromagnetic (or else 3D ferromagnetic) fluctuations [14], which give rise to a substantial enhancement of the effective mass and drive the system into a strong coupling regime of 3D antiferromagnetic fluctuations. In YRS, the quantum critical point is accessed by tuning the magnetic field. At the critical value of the field, the crossover from quasi-2D to 3D

antiferromagnetic fluctuations as a function of decreasing temperature takes place at $T = T_{cr}$. This crossover is clearly seen in experiment. Whereas in the quasi-2D AFM Gaussian fluctuation regime, marginal Fermi liquid (MFL) behavior [15] is observed experimentally (by this, we mean specific heat coefficient $\gamma(T) \propto \ln(T_0/T)$, resistivity $\rho(T) - \rho(0) \propto T$), in the critical regime the data are well-described by different power law dependences: $\gamma(T) \propto T^{\alpha-1}$, $\rho(T) - \rho(0) \propto T^\alpha$. These results follow only when the strongly anisotropic (\mathbf{k} -dependent) contribution of AFM fluctuations to the quasiparticle energy is smeared over the Fermi surface by sufficiently strong impurity scattering (elastic mean free path shorter than inelastic mean free path).

Critical quasiparticle picture. Our starting point is an Anderson lattice model of correlated f -electrons (spin σ , site i ; operators $f_{i\sigma}$) hybridizing with conduction electrons ($c_{\mathbf{k}\sigma}$), as described by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + \sum_{i,\sigma} \epsilon_f n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\mathbf{k},i,\sigma} (e^{i\mathbf{k}\mathbf{R}_i} c_{\mathbf{k}\sigma}^\dagger f_{i\sigma} + h.c.).$$

The single particle Green's functions $G_{ab}(\mathbf{k}, \omega)$, $a, b = \{c, f\}$, may be decomposed into a quasiparticle term and an incoherent contribution, $G(\mathbf{k}, \omega) = zG^q + G^{inc}$, where the quasiparticle weight factor z is defined by $z^{-1} = 1 - \partial \text{Re} \Sigma(\omega) / \partial \omega|_{\omega=E_k}$. Here $\Sigma(\omega)$ is the f -electron self energy generated from the Coulomb repulsion U and which we take to be \mathbf{k} -independent. In the limit of large U and close to half-filling ($n_f \lesssim 1$ electrons per site), one expects $z \ll 1$, leading to a large effective quasiparticle mass ratio $z^{-1} = m^*/m$. We assume that the Fermi level (at $k = k_F$) intersects the lower band, (see Fig. 1). Then the quasiparticle energy is given by $E_k^- = (m/m^*)v_F(k - k_F)$, where $v_F = 2(V/\epsilon_{k_F})^2 v_F^0$ is the Fermi velocity of the uncorrelated hybridized band and the quasiparticle width is $\Gamma = z \text{Im} \Sigma(E_k^-)$. That is to say $G^q(\mathbf{k}, \omega) = [\omega - E_k^- - i\Gamma]^{-1}$.

The condition for the quasiparticle picture to be valid is $\Gamma < |E_k^-|$. In the Fermi liquid regime, $\Gamma = c(E_k^-)^2 \ll |E_k^-|$ in the limit $E_k^- \rightarrow 0$. Here, we argue that the quasiparticle stability condition may be even satisfied in non-Fermi liquid situations. We extend the usual quasiparticle picture by allowing the parameter $z = m/m^*$ to depend on the energy scale, $z = z(\omega) = 1/[1 - \partial \Sigma(\omega) / \partial \omega]$. It is important to observe that the (retarded) self energy is an analytic function in the upper half plane, so that the real and imaginary parts of any nonanalytic term (in the lower half plane) are locally connected. A case of particular interest is the MFL form of the retarded self energy at $T = 0$ [15]: $\Sigma(\omega) = c_1[\omega \ln |\omega|/\omega_c - i(\pi/2)|\omega|]$, yielding the ratio $\Gamma/|E_k^-| = \pi/(2 \ln |\omega_c/E_k^-|) \ll 1$. Thus quasiparticles are still well defined in a MFL. Even in a true non-Fermi liquid phase with $\Sigma(\omega) \propto -i(i|\omega|)^\alpha$, $\alpha < 1$ so that $\text{Im} \Sigma(\omega) \propto \text{Re} \Sigma(\omega) \propto |\omega|^\alpha$ and $z \propto (|E_k^-|)^{1-\alpha}$,

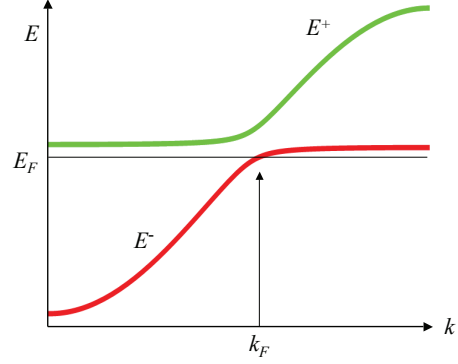


FIG. 1. Hybridized bands of the Anderson lattice model. Near half filling, the Fermi level E_F is near the top of the lower band.

one finds $\Gamma/|E_k^-| = \cot(\frac{\pi}{2}\alpha) < 1$ for $\frac{1}{2} < \alpha < 1$. These examples make clear that even if $z = 0$ at the Fermi surface, the spectral function for non-zero excitation energy may be peaked sharply enough to separate a quasiparticle contribution from the incoherent part.

Spectrum of antiferromagnetic spin fluctuations. We shall assume that in the heavy-quasiparticle paramagnetic phase, the self energy for the single particle Green's function is determined by the interaction with magnetic fluctuations. Here, we model the imaginary part of the renormalized retarded dynamical spin susceptibility for wave vectors \mathbf{q} near the AFM ordering wave vector \mathbf{Q} by

$$\text{Im} \chi(\mathbf{q}, \nu) = \frac{(N_0/z)(\nu/v_F^* Q)}{[1 + F(Q) + z(\mathbf{q} - \mathbf{Q})^2 \xi_0^2]^2 + (\nu/v_F^* Q)^2}, \quad (1)$$

where N_0 is the bare density of states at the Fermi surface, $v_F^* = (m/m^*)v_F$ is the renormalized quasiparticle Fermi velocity, $\xi_0 \simeq k_F^{-1}$ is the microscopic AFM correlation length and $F(Q)$ is a dimensionless generalized Landau parameter, with $F(Q) \rightarrow -1$ at the critical point. The factor z multiplying $(\mathbf{q} - \mathbf{Q})^2$ in Eq. (1) arises as follows: Consider the small $(\mathbf{q} - \mathbf{Q})$ expansion of the unscreened static quasiparticle susceptibility $\chi \sim (N_0/z)[1 - a(\mathbf{q} - \mathbf{Q})^2 \xi^2]$. The $(\mathbf{q} - \mathbf{Q})^2$ correction is governed by high-energy contributions and should not be renormalized, which leads to $a = z = m/m^*$. Note that the physical correlation length $\xi = \xi_0[(m^*/m)(1 + F(Q))]^{-1/2}$ diverges when the critical point is approached in any direction. As described above, we shall assume $m/m^* = z = z(\mathcal{E})$, where \mathcal{E} is the relevant energy scale, e.g. temperature T or magnetic field H (more precisely the Zeeman splitting), whichever is larger.

Quasiparticle self-energy. Now we set up a self-consistent determination of the quasiparticle self energy via the leading term in a skeleton graph expansion. Thus,

the quasiparticle width is given by

$$\Gamma(\omega) = \lambda^2(Q) \int \frac{d\nu}{\pi} \sum_{\mathbf{q}} \text{Im} G^{qp}(\mathbf{k} - \mathbf{q}, \omega - \nu) \text{Im} \chi(\mathbf{q}, \nu) \times [b(\nu) - f(\omega - \nu)], \quad (2)$$

where $\lambda(Q) = zF(Q)/N_0$ is the dimensionful (Landau) interaction vertex and $f(\omega), b(\omega)$ are Fermi and Bose functions, which at low T confine the ν -integration to the interval $[0, \omega]$. This is an equation of self consistency since $\Gamma = z\text{Im}\Sigma$ appears non-linearly in the integrand.

We consider 3D spin fluctuations and account for impurity scattering by averaging the right hand side of Eq. (2) over the Fermi surface. Near the critical line, $F(Q) \approx -1$, and for Q of order k_F , we find

$$\Gamma(\omega) = (4/9)(k_F \xi_0)^{-3} (v_F Q)^{-1/2} z^{-2} \omega^{3/2} \quad (3)$$

The dependence $\Gamma(\omega) \propto \omega^{3/2}$ in the case of 3D AFM fluctuations is well known. The structure of the full self energy $\Sigma(\omega) = \Gamma(\omega)/z$ may be determined from this result as $\Sigma(\omega) \propto (i\omega)^{3/2}/z^3(\omega)$. Here we have generalized to the frequency dependent z -factor. We may take a power law form $z(\omega) = b\omega^\alpha$. This enables the self-consistent determination of $z(\omega) = (1 - \partial \text{Re}\Sigma/\partial \omega)^{-1}$:

$$z^{-1}(\omega) = 1 + c'_3(k_F \xi_0 b)^{-3} (v_F Q)^{-1/2} 3(1/2 - \alpha) \omega^{1/2-3\alpha} \\ = 1 + c_3(k_F \xi_0)^{-3} (v_F Q)^{-1/2} z^{-3}(\omega) \omega^{1/2} \quad (4)$$

where c_3 is $O(1)$. We explore the consequences of the scale dependent z . For frequencies less than the temperature, we replace ω by T . Since $c_3(k_F \xi_0)^{-3} \approx 1$, we can say that as long as $z^{-3}(T)(T/v_F Q)^{1/2} \ll 1$ for any T , the system will be in the Gaussian fluctuation regime all the way down to the critical point. If however, the initial value of $z^{-1}(T)$, when one enters the 3D AFM fluctuation regime, is sufficiently large, such that $z^{-3}(T)(T/v_F Q)^{1/2} \gg 1$, a new regime is accessed, which is of a strong-coupling nature. We find the characteristics of this new regime within the present approximation by solving the self-consistent Eq. (4), to get

$$z(T) = [c_3(k_F \xi_0)^{-3}]^{1/2} (T/v_F Q)^{1/4}. \quad (5)$$

In the case of only 3D AFM fluctuations it is difficult to satisfy the strong-coupling condition unless $z^{-1}(T)$ is sufficiently large. Therefore, if on the initial approach to the critical point, fluctuations dominate that lead to a growing $z^{-1}(T)$ with decreasing T , the condition may be met at some point. The precise crossover point is determined by the crossover of these precursor fluctuations to the critical 3D AFM fluctuations and by the condition above that leads to Eq. (5). As mentioned in the introduction, there are clear indications in the data on YbRh_2Si_2 of both quasi-2D AFM and 3D FM fluctuations. In both cases one finds $z^{-1}(T) \propto \ln(T_0/T)$, so

that z^{-1} grows as $T \rightarrow 0$ and is about 40 in the heavy Fermi liquid region of the phase diagram.

Specific heat and electrical resistivity. Within the approximation of neglecting the momentum dependence of the self-energy, the entropy density is given by $S/V = (2N_0/T) \int d\omega \omega (-\partial f/\partial \omega) [\omega - \text{Re} \Sigma(\omega)]$. Substituting the power law dependence found above, $\text{Re} \Sigma(\omega) \propto |\omega|^{3/4} \text{sign}(\omega)$, we find a specific heat coefficient diverging in the limit $T \rightarrow 0$,

$$\gamma(T) = c_\gamma N_0 (T/v_F Q)^{-1/4} \quad (6)$$

A comparison of the theoretical temperature dependence of Eq. (6) with experiment [17] is shown in Fig. 2. To achieve this excellent fit, a T -independent constant specific heat has to be added. Such a term could arise from very low frequency ($\omega \ll T$) oscillators. Its magnitude represents about 0.4% of the total number of formula units. A possible source of such low frequency oscillators is spatially and temporally fluctuating AFM domains that oscillate about the preferred c -direction. An anisotropic exchange interaction has been proposed to explain the observed electron spin resonance g -shift [18]. We estimate the corresponding oscillator quantum as $\hbar\omega \approx 0.5\sigma$ K, where $\sigma \ll 1$ is the staggered magnetization per formula unit of a typical domain.

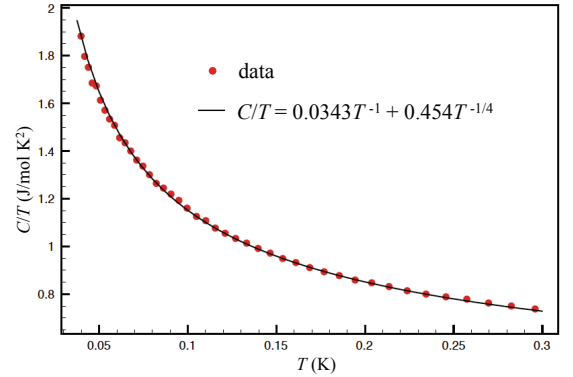


FIG. 2. Specific heat: Comparison of theory, Eq. (6) and data of Ref. [17] at the critical magnetic field and below the critical temperature for quantum critical scaling.

As mentioned above, beyond the critical regime proper, at temperatures $T > T_{cr} \approx 0.3\text{K}$, the data on YRS indicate the existence of Gaussian fluctuations of quasi-2D AFM or 3D FM character. This leads to $\gamma(T) = c_G N_0 (\partial/\partial T) [T \ln(T_h/(T + T_{FL}))]$, where T_{FL} is the crossover temperature into the Fermi liquid regime and $T_h \approx 20\text{K}$ is a high temperature cutoff scale of the order of the lattice Kondo temperature.

The electrical resistivity in the presence of impurity scattering may be obtained from the quasiparticle relaxation rate Γ as $\rho(T) = \rho(0) + c'_\rho (m/e^2 n) (m^*/m) \Gamma$. Using the above results in the scaling regime we find

$$\rho(T) - \rho(0) = c_\rho (m/e^2 n) (v_F Q)^{1/4} T^{3/4} \quad (7)$$

Upon entering the Gaussian fluctuation regime at $T > T_{cr}$ this fractional power law behavior crosses over into a linear T -dependence. A comparison of the theoretical temperature dependence of Eq. (7) with experiment [19] at the critical magnetic field is shown in Fig. 3.

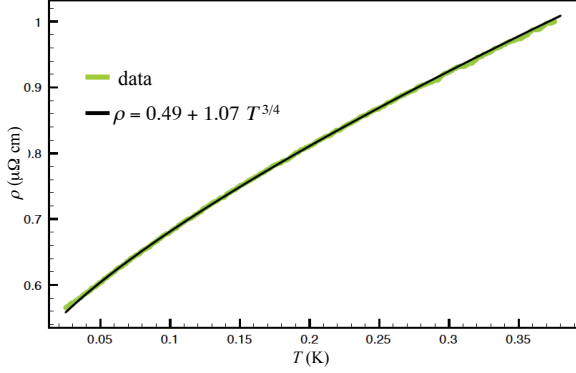


FIG. 3. Resistivity: Comparison of theory, Eq. (7) and data of Ref. [19] at the critical magnetic field and below the critical temperature for quantum critical scaling.

Local susceptibility. The local (q -integrated) susceptibility $\chi_{loc}(\omega)$ determines the nuclear spin relaxation time T_1 through the relation

$$\frac{1}{T_1 T} \propto \left[\frac{1}{\omega} \text{Im} \chi_{loc}(\omega) \right]_{\omega \approx 0} = \sum_{\mathbf{q}} \frac{1}{v_F Q \xi_0^4} \frac{N_0(m^*/m)^2}{[\xi^{-2} + q^2]^2} \\ = N_0(m^*/m)^4 (\xi/\xi_0) / (8\pi v_F Q \xi_0^3).$$

where ξ is the physical spin correlation length already defined below Eq. (1) as $\xi = \xi_0[(m^*/m)(1 + F(Q))]^{-1/2}$ and we used Eq. (1). Close to, but not quite at the critical point, such that $\lim_{T \rightarrow 0}(1 + F(Q)) > 0$, we then find

$$\frac{1}{T_1 T} \propto \left(\frac{m^*}{m} \right)^{7/2} = z^{-7/2} \sim T^{-7/8}. \quad (8)$$

Exactly at the critical point the temperature dependence of the control parameter enters, $[1 + F(Q)] \propto T^\beta$, and $1/T_1 T \propto T^{-7/8-\beta/2}$; the value of β is not known at present. Eq. (8) is a prediction of our theory; unfortunately the lowest field used in the available data [20], 0.15 T, is about twice the critical field of 0.06 T and is thus outside the critical region

Conclusion. We have presented a critical quasiparticle theory of heavy fermion compounds near a critical point. We focused on YbRh_2Si_2 , but the general framework of our approach should be applicable to other systems. The starting point is the observation that quasiparticles are well-defined in certain classes of non-Fermi liquid states. The best known example is the marginal Fermi liquid, properties of which are observed in a certain region of the $T - H$ phase diagram of YRS. Close to the critical point, however, much stronger deviations from Fermi liq-

uid theory are observed. We argue that the MFL behavior is caused by Gaussian fluctuations of quasi-2D antiferromagnetic and/or 3D ferromagnetic character. These fluctuations lead to a quasiparticle effective mass m^* increasing logarithmically with temperature. By contrast, 3D antiferromagnetic fluctuations do not lead to an increasing m^* , unless m^* exceeds a certain threshold. Then a strong coupling regime is reached. We calculated the critical exponents in that regime in a skeleton graph approach. Results for specific heat, resistivity and NMR relaxation rate are in Eqs. (6-8). In Figs. 2,3, we compare our results with the low- T data on specific heat and resistivity and find reasonable agreement.

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